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ON THE NUMERICAL INTEGRATION OF THE NEUTRON TRANSPORT EQUATION

by

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Abstract

A procedure for the direct numerical integration of the steady-state, elastic scattering neutron transport equation is presented. Conditions for the existence, uniqueness and non-negativeness of the numerical solution are obtained. Under these conditions it is shown that the scheme is stable and the numerical solution converges, with refinement of the mesh, to the solution of the transport equation.

Section 1. Introduction

A procedure for the direct numerical integration of the one-space-dimensional transport equation has been derived and tested. The success of these computations has made a general description of the method desirable. Thus the particular case of a multi-region, infinite plane shield is considered here as an illustration of the general technique.

The method is practical for steady state problems in which: 1) diffusion theory is not applicable, 2) slowing down by elastic scattering is important, 3) finite geometry, internal boundaries, or varying composition are present. Anisotropic or inelastic effects, which permit the integration of the birth integrals in section 2, may also be included. If either the spatial, angular or energy dependence may be eliminated the method becomes practical for various reactor calculations (i.e. for a particular Fourier component of the flux in a slab reactor).

The finite difference equations and an explicit solution procedure are given in sections 4 and 5. Here sufficient conditions on the mesh spacing are obtained to insure that the numerical equations have a unique, positive solution. For practical computations it is believed that these conditions may be relaxed.

In sections 6 and 7 we show that the numerical scheme is stable and convergent. This means that "small" errors introduced at the boundaries influence the solution only by a "small" amount; and by taking a sufficiently fine mesh the numerical solution can be made as "close" as we please to the true transport solution. The conditions under which this is true are the same as those which are sufficient for the solubility of the equations. Although the convergence characteristics of any method are of central importance in determining its practicality, this property is generally taken for granted, without any proof. This matter is treated in section 7; the method of proof also furnishes a bound on the error which, although pessimistic, may in some cases be useful.

Section 2. The Transport Equation

The steady state transport equation for neutrons with elastic scattering and isotropic source (i.e. linearized Boltzmann) is

$$(2.0)\quad [\underset{\sim}{\nabla}\cdot\underset{\sim}{\Omega} + \sigma^T(\underset{\sim}{r},u)]\psi(\underset{\sim}{r},\underset{\sim}{\Omega},u) = \sum_i b^{(i)}[\psi(\underset{\sim}{r},\underset{\sim}{\Omega},u)] + \frac{1}{4\pi}S(\underset{\sim}{r},u)\ ;$$

where

$$2.1 \quad b^{(i)}[\psi(\underset{\sim}{r},\underset{\sim}{\Omega},u)] = \int_{\max\left\{\begin{smallmatrix}0\\ u-q_i\end{smallmatrix}\right.}^{u} du'\sigma_i^S(\underset{\sim}{r},u') \int_{4\pi} d\underset{\sim}{\Omega}' F^{(i)}(\underset{\sim}{\Omega}:\underset{\sim}{\Omega}',u,u')\psi(\underset{\sim}{r},\underset{\sim}{\Omega}',u').$$

A discussion of this equation is contained in [1] and the notation used is as follows:

D1 $\underset{\sim}{r}$ = position vector of neutrons in the shield or reactor;

D2 $\underset{\sim}{\Omega}$ = unit vector in the direction of neutron velocity;

D3 $u = \ln {}^{E\,max}/_{E}$, lethargy variable defined in terms of the maximum source energy;

D4 $\psi(\underset{\sim}{r},\underset{\sim}{\Omega},u)$ = neutron flux (= $vN(\underset{\sim}{r},\underset{\sim}{\Omega},u)$, where v is the neutron speed and N is the neutron density in $(\underset{\sim}{r},\underset{\sim}{\Omega},u)$ space);

D5 $\sigma^T(\underset{\sim}{r},u)$ = total cross-section;

D6 $\sigma_i^S(\underset{\sim}{r},u)$ = scattering cross-section of the i-th scatterer;

D7 A_i = atomic weight of the i-th scatterer;

D8 $q_i = 2\ln\frac{A_i+1}{A_i-1}$, maximum lethargy degradation for neutrons on collision with nuclei of the i-th scatterer;

D9 $\alpha_i(u-u') = \frac{1}{2}\left[(A_i+1)\,e^{\frac{u-u'}{2}} - (A_i-1)e^{\frac{u'-u}{2}}\right]$, cosine of the scattering angle in the lab system for

elastic scattering from the i-th scatterer with lethargy degradation u-u';

D10 $F^{(i)}(\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}', u, u') \equiv$

$$\frac{(A_i+1)^2}{4\pi A_i} P_i(\alpha_i(u-u'), u')e^{u'-u}\delta[\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}' - \alpha_i(u-u')],$$

probability that a neutron scatter from $(\underset{\sim}{\Omega}', u')$ to $(\underset{\sim}{\Omega}, u)$ on collision with the i-th scatterer (for low energies, $u' >> 0$, and frequently for light scatterers it is usually assumed that $p_i(\alpha_i, u') = {}^1/2$);

D11 $S(\underset{\sim}{r}, u) \equiv$ flux of source neutrons.

The sum over i in (2.0) is assumed to include all elements present at position $\underset{\sim}{r}$. The source term, which is discussed in the next section, is assumed known. This essentially restricts the present considerations to shielding problems. A further restriction is imposed upon the geometry and symmetry of the problem as follows: define

$$\mu \equiv \frac{\underset{\sim}{r}}{|\underset{\sim}{r}|} \cdot \underset{\sim}{\Omega}, \tag{2.2}$$

the cosine of the angle between the position vector of a neutron and its velocity vector. It is then assumed that the flux has the functional dependence

$$\psi(\underset{\sim}{r}, \underset{\sim}{\Omega}, u) = \psi(\underset{\sim}{r}, \mu, u) . \tag{2.3}$$

This assumption is valid in at least two important

cases: first infinite plane geometries in which all spatial variations depend upon one coordinate, say x; and second, spherically symmetric geometries in which all spatial variations depend upon the radius, r. In the plane case, which will be the main consideration of this paper, (2.0) becomes

$$(2.4)\quad [\mu\frac{\partial}{\partial x} + \sigma^T(x,u)]\psi(x,\mu,u) = \sum_i b^{(i)}[\psi(x,\mu,u)] + \frac{1}{4\pi}S(x,u) .$$

For spherically symmetric geometries we have

$$(2.5)\quad [\mu\frac{\partial}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial}{\partial\mu} + \sigma^T(r,u)]\psi(r,\mu,u) = \sum b^{(i)}[\psi(r,\mu,u)] + \frac{1}{4\pi}S(r,u) .$$

In either of these cases, or in general whenever (2.3) is valid, the "birth integrals" (2.0) may be simplified by explicitly carrying out one of the angular integrations. This can readily be done if we introduce the spherical coordinates

$$(2.6)\quad \left.\begin{aligned} \underset{\sim}{\Omega} &= (1,0,0) \\ \underset{\sim}{\Omega}' &= (\cos\theta', \sin\theta'\cos\phi', \sin\theta'\sin\phi') \\ \frac{\underset{\sim}{r}}{|\underset{\sim}{r}|} &= (\cos\theta, \sin\theta\cos\phi, \sin\theta\sin\phi) \end{aligned}\right\} , \begin{cases} 0\leq\theta, \theta'\leq\pi \\ 0\leq\phi, \phi'\leq 2\pi \end{cases} ,$$

in (2.1) to obtain, using (D10) and (2.3),

$$(2.7)\quad b^{(i)}[\psi] = \frac{1}{2}\int_{\max\{u-q_i\}}^{u} du' g_i(\underset{\sim}{r},u,u') \int_0^{2\pi} d\phi' \int_0^{\pi} d\theta' \sin\theta' \delta[\cos\theta' - a_i(u-u')]\psi(r,\mu',u').$$

For simplicity we have introduced

$$(D12)\quad g_i(\underset{\sim}{r},u,u') \equiv \frac{(A_i+1)^2}{2\pi A_i}\, \sigma_i^S(\underset{\sim}{r},u')p_i(a_i,u')e^{u'-u} \quad ;$$

and from (2.2) and (2.6)

$$(2.8)\quad \mu = \cos\theta \quad ,$$

$$\mu' = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi'-\phi) \ .$$

A standard theorem on δ-functions states

$$\delta[g(\xi)] = \sum_k \left| \frac{dg(\xi_k)}{d\xi} \right|^{-1} \delta(\xi-\xi_k) \quad ,$$

where the sum is over all the zeroes (assumed simple) of $g(\xi)$; and it is simple to verify that

$$\int_0^{2\pi} f(\cos[\phi'-\phi])d\phi' = \int_0^{2\pi} f(\cos\phi'')d\phi'' = 2\int_0^{\pi} f(\cos\phi''')d\phi''' \quad .$$

Using these results and (2.8) in (2.7) yields

$$(2.9)\quad b^{(i)}[\psi] = \int_{\max\{0,u-q_i\}}^{u} du' g_i(\underset{\sim}{r},u,u') \int_0^{\pi} d\phi\, \psi(r,\Phi_i u') \quad ,$$

where

$$(2.10)\quad \Phi_i \equiv \Phi_i(\mu,u,u',\phi) = \mu a_i(u-u') + [(1-\mu^2)(1-a_i^2(u-u'))]^{1/2}\cos\phi \ .$$

For purposes of the numerical treatment it is useful to introduce the integral operator

$$(2.11)\quad h^{(i)}[\psi(\underset{\sim}{r},\mu,u);u'] \equiv \int_0^{\pi} d\phi\,\psi(\underset{\sim}{r},\Phi_i,u')$$

where Φ_i is given in (2.10). The birth integrals, (2.9), can now be written as

$$(2.12)\quad b^{(i)}[\psi(r,\mu,u)] = \int_{\max\{0,\,u-q_i\}}^{u} du'\,g_i(r,u,u')\,h^{(i)}[\psi(r,\mu,u);u'] \ .$$

Section 3. Plane Symmetrical Shield

Consider an infinite plane isotropic source of neutrons, infinitesimally thin, perpendicular to the x-axis at the origin. Then the source term, (D11), is given by

$$(3.0)\qquad S(x,u) = \delta(x)f(u) \ ,$$

where f(u) is, say, the fission energy spectrum of neutrons with $f(u) = 0$ for $u<0$ and $f(u)\geq 0$ for $u\geq 0$ (see(D3)). Let this source be surrounded by a finite symmetric shield in the range $-a\leq x\leq a$, with composition a function of x only. Outside the shield we assume vacuum of infinite extent. This is obviously a case of infinite plane geometry in which condition (2.3) holds with $\underset{\sim}{r}$ replaced by x. The appropriate form of the transport equation is then given by (2.4), with the source (3.0), and the birth integrals (2.9) in which $\underset{\sim}{r}$ is to be replaced by x. We allow σ^T and g_i to be

piecewise continuous functions of x; thus the shield may be composed of layers of different composition and variable density.

At the vacuum-shield interfaces there can be no neutrons entering the shield, thus

$$(3.1)\quad \begin{aligned} &\psi(a,\mu,u) = 0\ , -1\leq\mu<0\ , \\ &\psi(-a,\mu,u) = 0, 1\geq\mu>0\ . \end{aligned}$$

From the symmetry of the problem it is clear that the flux must satisfy

$$(3.2)\qquad \psi(x,\mu,u) = \psi(-x,-\mu,u)\ .$$

With this result it is possible to eliminate the source from (2.4) and replace the above problem by one in the range $0\leq x\leq a$. Thus we integrate (2.4) with respect to x from $-\varepsilon$ to ε, apply the symmetry condition (3.2), and pass to the limit $\varepsilon \longrightarrow 0$. Since all spatial singularities in the cross-sections and flux are assumed integrable this yields

$$(3.3)\quad \psi(0,\mu,u) = \psi(0,-\mu,u) + \frac{1}{\mu} f(u).$$

The problem has now been reduced to solving

$$(3.4)\quad [\mu\frac{\partial}{\partial x} + \sigma^T(x,u)]\psi(x,\mu,u) = \sum_i b^{(i)}[\psi(x,\mu,u)]\ ;$$

subject to the boundary conditions, from (3.1) and (3.3),

$$(3.5)\quad \begin{aligned} &a)\psi(a,\mu,u) = 0,\ -1\leq\mu<0\ , \\ &b)\psi(0,\mu,u) = \psi(0,-\mu,u) + \frac{1}{\mu} f(u),\ 0\leq\mu\leq 1\ ; \end{aligned}$$

in the domain (see fig.II)

$$(3.6)\quad D_U:\ [0\leq x\leq a,\ -1\leq\mu\leq 1,\ 0\leq u\leq U]\ .$$

At the maximum source energy, $\dot{u} = 0$, the birth integrals (2.9) vanish and the flux of highest energy neutrons must satisfy, from (3.4),

$$(3.7)\quad [\mu\frac{\partial}{\partial x} + \sigma^T(x,u)]\psi(x,\mu,0) = 0\ ,$$

and the boundary conditions (3.5). The solution is easily shown to be

$$(3.8)\ \psi(x,\mu,0) = \begin{cases} 0 & ,-1\leq\mu<0 \\ & ,\ 0\leq x\leq a\ . \\ \frac{f(0)}{\mu}\exp[\frac{-1}{\mu}\int_0^x \sigma^T(\xi,0)d\xi], & 0<\mu\leq 1 \end{cases}$$

The singularities at $\mu = 0$ in (3.5)b) and (3.8) are due to the infinite extent of the source plane which consequently has an infinite flux of neutrons streaming along its surface. These singularities are untenable for the proposed numerical procedure and may be eliminated by introducing the "slightly anisotropic" source

$$(3.9)\quad S(x,\mu,u) = \begin{cases} \delta(x)\ \frac{|\mu|}{\mu_*}f(u)\ , & 0\leq|\mu|\leq\mu_* \\ \delta(x)f(u) & ,\ \mu_*\leq|\mu|\leq 1 \end{cases}\ .$$

Here $\cos^{-1}\mu_*$ is an arbitrarily small angle. This source differs from the isotropic source (3.0) only in a small

angular region where the isotropic distribution is replaced by a cosine distribution. The boundary conditions for this source become

$$\psi(a,\mu,u) = 0 \qquad , -1\leq\mu<0$$

$$(3.10) \qquad \psi(0,\mu,u) = \psi(0,-\mu,u) + \begin{cases} \frac{1}{\mu_*} f(u) & , 0\leq\mu\leq\mu_* \\ \frac{1}{\mu} f(u) & , \mu_*\leq\mu\leq 1 \end{cases}$$

The highest energy flux, which satisfies (3.7) and (3.10), is given by

$$\psi(x,\mu,0) = 0 \qquad , -1\leq\mu<0$$

$$(3.11) \qquad \psi(x,\mu,0) = \exp\left[\frac{-1}{\mu}\int_0^x \sigma^T(\xi,0)d\xi\right] \begin{cases} \frac{1}{\mu_*} f(0), & 0\leq\mu\leq\mu_* \\ \frac{1}{\mu} f(0), & \mu_*\leq\mu\leq 1 \end{cases} \quad 0\leq x\leq a \ .$$

The effect of the "slightly anisotropic" source is shown in fig.I where the highest energy flux in the source plane is plotted as a function of μ for both (3.8) and (3.11). The spatial dependence of $\psi(x,\mu,0)$ may be inferred by considering exponentially damped waves emanating from the appropriate $\psi(0,\mu,0)$ curve of fig.I. The rate of damping must increase as $\mu \longrightarrow 0$ through positive values.

In summary we seek the solution (assuming existence and uniqueness) of equation (3.4) subject to the boundary conditions (3.10) in the domain D_U of (3.6). The flux at highest energy in this solution is given by (3.11). From physical considerations the solution should be non-negative and continuous in x. The domain D_U is shown in

fig.II where the appropriate boundary conditions and highest energy solution are indicated.

Section 4. Finite Difference Approximation

In this section the problem formulated at the end of the previous section will be approximated by a set of finite difference equations. Thus on the domain D_U of (3.6) we introduce the mesh Δ_N defined by the points:

$$
(4.0)\quad
\begin{aligned}
&a)\, x_{r+1} = x_r + \Delta x_r\,,\ x_o = 0\,,\ x_R = a,\ (0 \le r \le R);\\
&b)\, \mu_{s+1} = \mu_s + \Delta\mu_s\,,\ \mu_o = -1, \mu_{S_1} < 0, \mu_{S_1+1} > 0, \mu_{S_2} = 1, (0 \le s \le S_2);\\
&c)\, u_{n+1} = u_n + \Delta u_n,\ u_o = 0\,,\ u_N = U\,,\ (0 \le n \le N);\\
&d)\, \phi_{j+1} = \phi_j + \Delta\phi_j,\ \phi_o = 0\,,\ \phi_J = \pi\,,\ (0 \le j \le J).
\end{aligned}
$$

Here the ϕ_j are values of the dummy integration variable in (2.9) or (2.11). All spacings Δx_r, $\Delta\mu_s$, Δu_n and $\Delta\phi_j$ are positive. The angular spacing (4.0)b) is chosen such that $\mu_s \neq 0$ for all s. This eliminates the consideration of a special set of difference equations for the case $\mu = 0$. The x-spacing, (4.0)a), is to be such that all interfaces (points of discontinuity of the cross-sections) coincide with mesh points. Values of functions which are known at points of Δ_N are denoted by

$$
(4.1)\quad
\begin{aligned}
&a)\, \sigma^T(r,n) \equiv \sigma^T(x_r, u_n)\,,\ \text{see (D5)};\\
&b)\, g_i(r,n,n') \equiv g_i(x_r, u_n, u_{n'})\,,\ \text{see (D12)};
\end{aligned}
$$

$$(4.1)\quad \begin{aligned} &c)\, f(n) \doteq f(u_n)\ , \text{ see } (3.0) \text{ and } (3.9); \\ &d)\, \Phi_i(s,n,n',j) \doteq \Phi_i(\mu_s, u_n, u_{n'}, \emptyset_j), \text{ see } (2.10). \end{aligned}$$

If x_r is a point of discontinuity of σ^T (or g_i) then (4.1)a) or b) is defined as follows:

$$(4.2)\quad \sigma^T(r,n) \doteq \left.\begin{cases} \sigma^T(x_r-0,u_n) \text{ if } \sigma^T(r-1,n) \\ \\ \sigma^T(x_r+0,u_n) \text{ if } \sigma^T(r+1,n) \end{cases}\right\} \begin{array}{l}\text{appears in the} \\ \text{difference equation} \\ \text{with } \sigma^T(r,n);\end{array}$$

(and similarly for g_i). This lack of single-valuedness of the cross-sections on Δ_N allows the limit of the numerical solution to be continuous and have discontinuous derivatives in x. The meaning of (4.2) is made clearer after (4.14).

With some aim at simplicity in the present treatment all integrals are approximated by the trapezoidal rule and only linear interpolations are used. Before applying these techniques it is useful to consider fig.III: a typical (μ,u)-plane at some fixed value of x, say $x = x_r$, in which the domain of integration for the i-th birth integral, (2.10)-(2.12), is indicated by the shaded region. The intersections of horizontal and vertical solid lines are points of the grid (4.0)b),c) for the fixed x_r. The dots represent locations of $\Phi_i(s,n,n',j)$, which function as the μ-argument in $\psi(x,\mu,u)$ (see (2.11)), for some fixed (s,n) and all

(n',j) in $0\leq j\leq J$, $n_i\leq n'\leq n$. Here, as indicated in the figure, n_i is defined as the integer such that

$$(4.3)\quad \begin{aligned} &u_{n_i}\leq\mu_n-q_i<u_{n_i+1}, \text{ for } u_n-q_i>0\ ,\\ &u_{n_i}=0 \qquad\qquad , \text{ for } u_n-q_i\leq 0\ . \end{aligned}$$

Let $W^n_{r,s}$ be the numerical approximation to the flux $\psi(x_r,\mu_s,u_n)$ on Δ_N. Then the integral operator (2.11) is approximated on the mesh by the difference operator $H^{(i)}[W^n_{r,s};n']\simeq h^{(i)}[\psi(x_r,\mu_s,u_n);u_{n'}]$, where

$$(4.4)\quad \begin{aligned} &\text{a)}\ H^{(i)}[W^n_{r,s};n'] \equiv \frac{1}{2}\sum_{j=0}^{J}\frac{\varepsilon_j}{\Delta\mu_{s_j}}\Big\{[\mu_{s_j+1}-\Phi_i(s,n,n',j)]W^{n'}_{r,s_j}+\\ &\qquad +[\Phi_i(s,n,n',j)-\mu_{s_j}]W^{n'}_{r,s_j+1}\Big\},\ n_i\leq n'<n;\\ &\text{b)}\ H^{(i)}[W^n_{r,s};n] \equiv \pi W^n_{r,s}\ . \end{aligned}$$

Here s_j is the integer such that*

$$(4.5)\quad \mu_{s_j}\leq\Phi_i(s,n,n',j)<\mu_{s_j+1}\ ,$$

and we have introduced

$$(4.6)\quad \varepsilon_j \equiv \begin{cases} \Delta\phi_0 & , j=0\\ \Delta\phi_{j-1}+\Delta\phi_j & , 1\leq j\leq J-1\\ \Delta\phi_{J-1} & , j=J \end{cases}$$

The definition (4.4)b) follows from the fact that $\alpha_i(u_n-u_n)=1$ and hence, $\Phi_i(s,n,n,j)=\mu_s$ for all j.

* There is obviously a dependence of s_j on i,n and n' which, for simplicity of notation, has been dropped. This is true also of the sets $L_{s'}$ and $R_{s'}$ about to be introduced.

For practical numerical procedures and for the stability analysis it is useful to write (4.4)a) as

$$(4.7)\quad H^{(i)}[W^{n}_{r,s};n'] = \sum_{s'=0}^{S_2} \omega_i(s,n,n',s')W^{n'}_{r,s'}\ ,\quad n_i \leq n' < n.$$

From (4.0)d) and (4.4)-(4.7) we must have

$$(4.8)\quad \omega_i(s,n,n',s') \equiv \frac{1}{2}\left\{\sum_{j\varepsilon L_{s'}} \frac{\varepsilon_j}{\Delta\mu_{s_j}}[\mu_{s_j+1}-\Phi_i(s,n,n',j)] + \right.$$

$$\left. + \sum_{j\varepsilon R_{s'}} \frac{\varepsilon_j}{\Delta\mu_{s_j}}[\Phi_i(s,n,n',j)-\mu_{s_j}]\right\}\ ,$$

where the disjoint sets $L_{s'}$ and $R_{s'}$ are defined by

$$(4.9)\quad \begin{aligned} L_{s'} &\equiv \left\{\text{all } j \text{ such that: } \mu_{s_j} = \mu_{s'}\right. \\ R_{s'} &\equiv \left\{\text{all } j \text{ such that: } \mu_{s_j+1} = \mu_{s'}\right. \end{aligned}\ ,\quad 0 \leq s' \leq S_2$$

Clearly, from the definitions (4.5) and (4.9), we have in the set theoretic sense

$$\sum_{s'=0}^{S_2}\left\{L_{s'}+R_{s'}\right\} = \left\{\text{all } j \text{ in: } 0 \leq j \leq J\right\}\ ,$$

which aids in confirming the identity of the sums (4.4)a) and (4.7). If some of the sets $\{L_{s'}+R_{s'}\}$ are empty, which may frequently be the case, the corresponding $\omega_i(s,n,n',s')$ vanish (see fig.III).

The birth integrals (2.12) are approximated on Δ_N by the difference operators $B^{(i)}[W^{n}_{r,s}] \approx b^{(i)}[\psi(x_r,\mu_s,u_n)]$, which are defined as

$$(4.10)\quad B^{(i)}[W^n_{r,s}] \equiv \frac{1}{2}\sum_{n'=n_i}^{n}\delta_i(n')g_i(r,n,n')H^{(i)}[W^n_{r,s};n'],\ n>0.$$

Here n_i is defined in (4.3), $H^{(i)}[W^n_{r,s};n']$ is defined in (4.4)-(4.6), $g_i(r,n,n')$ is defined in (4.1)b), and we have introduced

$$(4.11)\quad \delta_i(n') \equiv \begin{cases} \Delta u_{n-1} & ,n' = n \quad ; \\ \Delta u_{n'-1} + \Delta u_{n'} & ,n>n'>n_i + 1 \ ; \\ \Delta u_{n_i+1} + \Delta u_{n_i}\left[1-\left(\dfrac{u_n-q_i-u_{n_i}}{\Delta u_{n_i}}\right)^2\right] & ,n' = n_i + 1 \ ; \\ \Delta u_{n_i}\left[1-\left(\dfrac{u_n-q_i-u_{n_i}}{\Delta u_{n_i}}\right)\right]^2 & ,n' = n_i \quad . \end{cases}$$

In order to construct a solution of the equations being formulated and to analyze their stability it is useful to write (4.10) in the form

$$(4.12)\quad B^{(i)}[W^n_{r,s}] = \Delta u_{n-1}\,\frac{\pi}{2}g_i(r,n,n)W^n_{r,s} + \overline{B^{(i)}}[W^n_{r,s}],\ n>0\ ;$$

where we have used (4.4)b) and the definition

$$(4.13)\quad \overline{B^{(i)}}[W^n_{r,s}] \equiv \frac{1}{2}\sum_{n'=n_i}^{n-1}\delta_i(n')g_i(r,n,n')H^{(i)}[W^n_{r,s};n'],\ n>0.$$

It has been assumed here that $\Delta u_{n-1} \leq q_i$. If this is not the case Δu_{n-1} in (4.12) should be replaced by the $\delta_i(n_i+1)$ of (4.11). However it is felt that the present procedure should not be used (at least in its current form) in this case and thus (4.12) will be retained

throughout.

The difference equations, which are to approximate the transport equation (3.4) on Δ_N are chosen to be

$$\mu_s \frac{W^n_{r+1,s} - W^n_{r,s}}{\Delta x_r} + \frac{1}{2}\left[\sigma^T(r+1,n)W^n_{r+1,s} + \sigma^T(r,n)W^n_{r,s}\right]$$

(4.14)

$$= \frac{1}{2}\sum_i \left[B^{(i)}[W^n_{r+1,s}] + B^{(i)}[W^n_{r,s}]\right], \quad \begin{cases} 0 \le r \le R-1 \\ 0 \le s \le S_2 \\ 1 \le n \le N \end{cases}$$

The difference quotient is centered at $x_{r+1/2} = x_r + \frac{\Delta x_r}{2}$ and the other terms are taken as averages about this point. If there is a discontinuity in σ^T or g_i at some $x = x_r$ it is now clear that the value to be used for $\sigma^T(r,n)$ or $g_i(r,n,n')$ is that belonging to the medium containing the point about which the appropriate equation (4.14) is centered (see (4.2) and following). To these equations we adjoin the approximation to the highest energy flux

(3.11)

$$W^o_{r,s} = 0 \qquad , 0 \le s \le S_1;$$

(4.15)

$$W^o_{r,s} = \left(\exp\left[\frac{-1}{\mu_s}\sum_{r'=0}^{r-1}\frac{\Delta x_{r'}}{2}\left\{\sigma^T(r'+1,0)+\sigma^T(r',0)\right\}\right]\right)\begin{cases} \frac{f(0)}{\mu_*}, \text{all } s\ 3: \\ \quad \mu_{S_1} < \mu_s \le \mu_*; \\ \frac{f(0)}{\mu_s}, \text{all } s\ 3: \\ \quad \mu_* \le \mu_s \le \mu_{S_2} = 1; \end{cases}$$

for $0 \le r \le R$.

The boundary conditions (3.10) are approximated by

$$
(4.16)\quad
\begin{cases}
\text{a) } W^n_{R,s}=0 & ,\ 0\le s\le S_1\ ; \\
\text{b) } W^n_{o,s}=[(\mu_s+\mu_{\underline{s}+1})W^n_{o,\underline{s}}-(\mu_s+\mu_{\underline{s}})W^n_{o,\underline{s}+1}]\dfrac{1}{\Delta\mu_{\underline{s}}}+\begin{cases}\dfrac{f(n)}{\mu_*}, & \text{all } s\ 3: \\ & \mu_{S1}<\mu_s\le\mu_*; \\ \dfrac{f(n)}{\mu_s}, & \text{all } s\ 3: \\ & \mu_*\le\mu_s\le\mu_{S_2}=1.\end{cases}
\end{cases}
$$

Here we have defined $\underline{s}$ as the largest integer $\le S_1$ such that $\mu_{\underline{s}}\le-\mu_s$.

Section 5. Solution of the Difference Equations

In this section an explicit procedure for solving the difference equations (4.14)-(4.16) is presented. This provides a constructive proof of the uniqueness of the numerical solution which is required of any practical scheme and is necessary for the stability analysis. Sufficient conditions on the mesh spacing are presented which insure that the solution procedure is possible and that the numerical solution is non-negative.

We first note that equations (4.14)-(4.16), with (4.7) and (4.10), form a system of $(N+1)(R+1)(S_2+1)$ inhomogenous linear equations in as many unknowns, $W^n_{r,s}$. The solution of this system is obtained by an induction on n. To start the induction we note that the highest energy approximation, $W^o_{r,s}$, is given in (4.15) for all

r and s. Then assuming given the $W^{n'}_{r,s}$ for all $n' \leq n-1$ and $0 \leq r \leq R$, $0 \leq s \leq S_2$ we write (4.14) as

(5.0)

$$[\mu_s + \Delta x_r \beta(r+1,n)] W^n_{r+1,s} - [\mu_s - \Delta x_r \beta(r,n)] W^n_{r,s} = \frac{\Delta x_r}{2} \sum_i (B^{(i)}[W^n_{r+1,s}] + \overline{B^{(i)}}[W^n_{r,s}])$$

Here we have used (4.12) and (4.13), and introduced

$$(5.1) \quad 2\beta(r,n) \equiv \sigma^T(r,n) - \Delta u_{n-1} \frac{\pi}{2} \sum_i g_i(r,n,n) \ .$$

The inductive hypothesis insures, by (4.7) and (4.13), that the right side of (5.0) is known. For $s \leq S_1$, $W^n_{R,s} = 0$ by the boundary conditions (4.16)a). Then starting with $r = R-1$, and continuing recursively down to $r = 0$, equations (5.0) yield all $W^n_{r,s}$ for $0 \leq r \leq R-1$ and $s \leq S_1$. The values of $W^n_{o,s}$ so computed yield, by (4.16)b), all the $W^n_{o,s}$ for $s > S_1$. Another recursion, from $r = 0$ to $r = R-1$, in (5.0) yields the remaining $W^n_{r,s}$ for $1 \leq r \leq R$, $s > S_1$. This completes the induction.

The recursive solution of (5.0) is possible if

$$(5.2) \quad \left.\begin{array}{ll} \text{a)} & -\mu_s + \Delta x_r \beta(r,n) \neq 0 \ , \quad s \leq S_1 \\ \text{b)} & \mu_s + \Delta x_r \beta(r+1,n) \neq 0, \quad s > S_1 \end{array}\right\} 0 \leq r \leq R-1 \ ,$$

and the induction holds if these conditions are satisfied for all $n \geq 1$. With the much stronger conditions

$$(5.3)\quad \begin{cases} \text{a)} & \left.\begin{matrix} -\mu_s + \Delta x_r \beta(r,n) > 0 \\ -\mu_s - \Delta x_r \beta(r+1,n) \geq 0 \end{matrix}\right\} s \leq S_1 (\mu_s < 0) \\ \text{b)} & \left.\begin{matrix} \mu_s + \Delta x_r \beta(r+1,n) > 0 \\ \mu_s - \Delta x_r \beta(r,n) \geq 0 \end{matrix}\right\} s > S_1 (\mu_s > 0) \end{cases} , \quad \begin{cases} 0 \leq r \leq R-1 \\ 1 \leq n \leq N \end{cases} ,$$

it is easily proven that $W^n_{r,s} \geq 0$ on the entire mesh Δ_N. This proof relies on the fact that $\omega_i(s,n,n',j) \geq 0$, and $f(n) \geq 0$ for all i,n,n',s and j. The first of conditions (5.3)a) and b) are satisfied provided

$$(5.4)\quad \beta(r,n) \geq 0 \quad , \quad 0 \leq r \leq R \ , \ n \geq 1 \ .$$

These conditions imply (5.2) and hence the solvability of the difference equations. To examine condition (5.4) in more detail we use the definitions (5.1), (D12) and (D9) and recall from the definition of total cross-section that

$$(5.5)\quad \sigma^T(r,n) = \sum_i [\sigma_i^a(r,n) + \sigma_i^S(r,n)] .$$

This yields

$$(5.6)\quad \beta(r,n) \equiv \frac{1}{2} \sum_i \left\{ \sigma_i^a(r,n) + [1 - \Delta\mu_{n-1} \frac{(A_i+1)^2}{4A_i} p_i(1,n)] \sigma_i^S(r,n) \right\} .$$

where $\sigma_i^a(r,n)$ is the absorption cross-section of the i-th scatterer at (x_r, u_n) and $p_i(1,n) \equiv p_i(\alpha_i(u_n - u_n), u_n)$. The lethargy spacing may now be taken such that

$$(5.7)\quad \Delta u_{n-1} \leq [1 + \frac{\sigma_i^a(r,n)}{\sigma_i^S(r,n)}] \frac{4A_i}{(A_i+1)^2 p_i(1,n)} , \text{for all } i, r \text{ and } n>0;$$

in which case (5.4) is satisfied. When this condition is satisfied the second of (5.3)a) and b) are satisfied provided the spatial and angular spacing are chosen such that

$$(5.8)\quad \Delta x_r \leq \frac{2|\mu_s|}{\max[\beta(r,n),\beta(r+1,n)]}, \text{ for all } r,s \text{ and } n>0.$$

Conditions (5.7) and (5.8) are then sufficient for the existence and uniqueness of a non-negative numerical solution, $W^n_{r,s}$, on the mesh Δ_N. For practical computations these restrictions are no doubt too severe.

Section 6. Consistency of Difference Equations

In the present section we outline a proof of the consistency of the difference equations; that is, that the difference equations approach the transport equation as the mesh is refined. A trivial observation of consistency in the present case is obscured by the complexity of the equations. The present analysis also yields a bound on the truncation errors, which is required in the convergence proof.

Let $\psi(x,\mu,u)$ be any function satisfying (3.10) and (3.11) with differentiability properties in D_U which are to be specified as required. Then we introduce the linear transport operator $\mathcal{T}[\ ]$ by

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$$(6.0)\quad \mathcal{T}[\psi(x,\mu,u)] \equiv [\mu \frac{\partial}{\partial x} + \sigma^T(x,u)]\psi(x,\mu,u) - \sum_i b^{(i)}[\psi(x,\mu,u)],$$

where $b^{(i)}[\psi]$ is defined by (2.11) and (2.12). The difference equations are represented by the linear difference operator,

$$(6.1)\quad t[\psi(x_r + \frac{\Delta x_r}{2}\mu_s, u_n)] \equiv \mu_s \frac{\psi^n_{r+1,s} - \psi^n_{r,s}}{\Delta x_r} + \frac{1}{2}\Big\{\sigma^T(r+1,n)\psi^n_{r+1,s} +$$

$$+ \sigma^T(r,n)\psi^n_{r,s}\Big\} - \frac{1}{2}\sum_i B^{(i)}[\psi^n_{r+1,s}] + B^{(i)}[\psi^n_{r,s}] \quad ,$$

where $\psi^n_{r,s} \equiv \psi(x_r, \mu_s, u_n)$, the mesh is Δ_N defined by (4.0), and the $B^{(i)}[\psi]$ are defined in (4.4) and (4.10). The values of $\sigma^T(r,n)$ (and $g_i(r,n,n')$) at points $x = x_r$ of discontinuity are defined by (4.2). We define the truncation, $T^n_{r,s}$, on Δ_N by

$$(6.2)\quad (\mathcal{T}-t)[\psi(x_r + \frac{\Delta x_r}{2}, \mu_s, u_n)] \equiv T^n_{r,s} \quad ,$$

for the given function ψ. The difference operator, t, is said to be consistent with the transport operator, $\mathcal{T}$, for the given ψ if

$$(6.3)\quad T^n_{r,s} \longrightarrow 0 \text{ as } \max(\Delta x_r, \Delta\mu_s, \Delta u_n, \Delta\phi_j) \longrightarrow 0 \text{ on } \Delta_N \, .$$

The proof proceeds from an evaluation of the truncation by standard methods.

From the usual Taylor expansions we obtain

a) $\frac{\partial}{\partial x}\psi^n_{r+1/2,s} - [\frac{\psi^n_{r+1,s} - \psi^n_{r,s}}{\Delta x_r}] = \frac{-\Delta x_r^2}{6} \frac{\partial^3}{\partial x^3}\psi(x_r + \theta \Delta x_r, \mu_s, u_n)$

(6.4)

b) $\sigma^T(r+1/2,n)\psi^n_{r+1/2,s} - \frac{1}{2}[\sigma^T(r+1,n)\psi^n_{r+1,s} + \sigma^T(r,n)\psi^n_{r,s}] =$

$$= \frac{-\Delta x_r^2}{2} \frac{\partial^2}{\partial x^2}[\sigma^T(x_r + \theta \Delta x_r, u_n)\psi(x_r + \theta \Delta x_r, \mu_s, u_n)]$$

Here we have used the obvious notation, $\psi^n_{r+1/2,s} \equiv \psi(x_r + \frac{\Delta x_r}{2}, \mu_s, u_n)$; and the assumptions that $\frac{\partial^3 \psi}{\partial x^3}$ and $\frac{\partial^2[\sigma^T \psi]}{\partial x^2}$ are continuous functions of x in each interval $[x_{r+1} - x_r]$. The contributions to $T^n_{r,s}$ from the birth integral approximations are obtained from the identity

(6.5) $b[\psi^n_{r+1/2,s}] - \frac{1}{2}[B[\psi^n_{r+1,s}] + B[\psi^n_{r,s}]] \equiv b[\psi^n_{r+1/2,s}] -$

$$- \frac{1}{2}[b[\psi^n_{r+1,s}] + b[\psi^n_{r,s}]] + \frac{1}{2}[(b[\psi^n_{r+1,s}] - B[\psi^n_{r+1,s}])$$

$$+ (b[\psi^n_{r,s}] - B[\psi^n_{r,s}])] .$$

The superscript i has been temporarilly dropped for simplicity. As in (6.4)b) we now have

(6.6) $b[\psi^n_{r+1/2,s}] - \frac{1}{2}[b[\psi^n_{r+1,s}] + b[\psi^n_{r,s}]] =$

$$= \frac{-\Delta x_r^2}{2} \frac{\partial^2}{\partial x^2} b[\psi(x_r + \theta \Delta x_r, \mu_s, u_n)] ,$$

with proper continuity assumptions on $\frac{\partial^2 b}{\partial x^2}$. The remaining terms in (6.5) are, by (2.12) and (4.10),

$$(6.7)\quad b[\psi^n_{r,s}]-B[\psi^n_{r,s}]=\sum_{n'=n_i}^{n-1}\int_{u_{n'}}^{u_{n'}+\Delta u_{n'}} du'\Big\{g(x_r,u_n,u')h[\psi^n_{r,s};u']-$$

$$-\tfrac{1}{2}(g(r,n,n'+1)H[\psi^n_{r,s},n'+1]+g(r,n,n')H[\psi^n_{r,s},n'])\Big\}.$$

In order to avoid a special case of no particular difficulty we have here assumed $u_n-q_i = u_{n_i}$. The above integrand can be rewritten as

$$(6.8)\quad \Big\{\ -\ \Big\}\equiv g(x_r,u_n,u')h[\psi^n_{r,s};u']-\tfrac{1}{2}(g(r,n,n'+1)h[\psi^n_{r,s};n'+1]+$$
$$+g(r,n,n')h[\psi^n_{r,s};n'])$$
$$+\tfrac{1}{2}g(r,n,n'+1)(h[\psi^n_{r,s};n'+1]-$$
$$-H[\psi^n_{r,s};n'+1])$$
$$+\tfrac{1}{2}g(r,n,n')(h[\psi^n_{r,s};n']-$$
$$-H[\psi^n_{r,s};n'])\quad .$$

An expansion similar to that of (6.4)b) (but with respect to u' in the first two terms on the right of (6.8) yields

$$(6.9)\quad \int_{u_{n'}}^{u_{n'}+\Delta u_{n'}} du'\Big\{g(x_r,u_n,u')h[\psi^n_{r,s};n']-\tfrac{1}{2}(g(r,n,n'+1)h[\psi^n_{r,s};n'+1]+$$

$$+g)r,n,n')h[\psi^n_{r,s},n'])\Big\}=$$

$$=\frac{(\Delta u_{n'})^2}{4}\left.\frac{\partial g(x_r,u_n,u')h[\psi^n_{r,s};u']}{\partial u'}\right|_{u'=u_{n'}+\Delta u_{n'}}^{u'=u_{n'}}+\mathcal{O}(\Delta u^3_{n'}).$$

The remaining terms in (6.8) are evaluated from the definitions (2.11) and (4.4)-(4.6) which yield

$$(6.10)\quad h[\psi^{n}_{r,s};n']-H[\psi^{n}_{r,s};n']=\sum_{j=0}^{J-1}\int_{\phi_j}^{\phi+\Delta\phi_j} d\phi\Big\{\psi(x_r,\Phi(\mu_s,u_n,u_{n'},\phi),u_{n'})$$

$$-\frac{1}{2}[\psi(x_r,\Phi(\mu_s,u_n,u_{n'},\phi_j),u_{n'})+\psi(x_r,\Phi(\mu_s,u_n,u_{n'},\phi_{j+1}),u_{n'})]\Big\}$$

$$+\frac{1}{2}\sum_{j=0}^{J-1}\Delta\phi_j\Big\{\psi(x_r,\Phi(\mu_s,u_n,u_{n'},\phi_j),u_{n'})-[\frac{\mu_{s_j+1}-\Phi(\mu_s,u_n,u_{n'},\phi_j)}{\Delta\mu_{s_j}}\psi^{n'}_{r,s_j}$$

$$+\frac{\Phi(\mu_s,u_n,u_{n'},\phi_j)-\mu_{s_j}}{\Delta\mu_{s_j}}\psi^{n'}_{r,s_j+1}]\Big\}+\frac{1}{2}\sum_{j=0}^{J-1}\Delta\phi_j\Big\{\psi(x_r,\Phi(\mu_s,u_n,u_{n'},\phi_{j+1}),u_{n'})-$$

$$-[\frac{\mu_{s_{j+1}+1}-\Phi(\mu_s,u_n,u_{n'},\phi_{j+1})}{\Delta\mu_{s_{j+1}}}\psi^{n'}_{r,s_{j+1}}$$

$$+\frac{\Phi(\mu_s,u_n,u_{n'},\phi_{j+1})-\mu_{s_{j+1}}}{\Delta\mu_{s_{j+1}}}\psi^{n'}_{r,s_{j+1}+1}]\Big\}$$

The usual Taylor expansions are now used above to obtain

$$(6.11)\quad h[\psi^{n}_{r,s};n']-H[\psi^{n}_{r,s};n']=$$

$$=\sum_{j=0}^{J-1}\Big\{\frac{(\Delta\phi_j)^2}{4}\frac{\partial\psi(x_r,\Phi,(\mu_s,u_n,u_{n'},\phi),u_{n'})}{\partial\phi}\Bigg|_{\phi=\phi_{j+1}}^{\phi=\phi_j}+\sigma(\Delta\phi_j^3)\Big\}$$

$$+\sum_{j=0}^{J-1}\Delta\phi_j\Big\{\frac{(\Delta\mu_{s_j})^2}{4}[\frac{\mu_{s_j+1}-\Phi(\mu_s,u_n,u_{n'},\phi_j)}{\Delta\mu_{s_j}}\frac{\Phi(\mu_s,u_n,u_{n'},\phi_j)-\mu_{s_j}}{\Delta\mu_{s_j}}]\frac{\partial\psi^{n}_{r,\bar{s}_j}}{\partial\mu}$$

$$+\frac{(\Delta\mu_{s_{j+1}})^2}{4}[\frac{\mu_{s_{j+1}+1}-\Phi(\mu_s,u_n,u_{n'},\phi_{j+1})}{\Delta\mu_{s_{j+1}}}\frac{\Phi(\mu_s,u_n,u_{n'},\phi_j)-\mu_{s_{j+1}}}{\Delta\mu_{s_{j+1}}}]\frac{\partial\psi^{n}_{r,\bar{s}_{j+1}}}{\partial\mu}\Big\}$$

Here we have introduced $\psi^n_{r,\bar{s}_j} = \psi(x_r, \mu_{s_j} + \theta\Delta\mu_{s_j}, u_n)$ for some $0 \leq \theta \leq 1$. Using (6.4)-(6.11) in (6.2) we may obtain an expression for $T^n_{r,s}$. Since this result is rather cumbersome we present instead a bound on the truncation which is obtained from the complete expression. Thus we let

$$(6.12)\quad \Delta x = \max_r \Delta x_r, \Delta u = \max_n \Delta u_n, \Delta\mu = \max_s \Delta\mu_s, \Delta\phi = \max_j \Delta\phi_j,$$

and then

$$(6.13)\quad \left|T^n_{r,s}\right| < (\Delta x)^2\alpha + (\Delta\mu)^2\beta + (\Delta u)\gamma + (\Delta\phi)\delta + \sigma(\Delta u^2 + \Delta\phi^2) \quad .$$

Here α, β, γ and δ are independent of the mesh spacing and depend only upon the cross-sections and particular function ψ and their derivatives in D_U. Explicitly we have defined

$$\alpha = \frac{1}{2}\left\{\frac{1}{3}\max_{D_U}\left|\frac{\partial^3\psi}{\partial x^3}\right| + \max_{D_U}\left|\frac{\partial^2\sigma^T\psi}{\partial x^2}\right| + \sum_i \max_{D_U}\left|\frac{\partial^2 b^{(i)}[\psi]}{\partial x^2}\right|\right\}$$

$$\beta = \frac{\pi}{8}\left\{\sum_i q_i \max_{D_U} g_i \cdot \max_{D_U}\left|\frac{\partial\psi}{\partial\mu}\right|\right\}$$

(6.14)

$$\gamma = \frac{1}{2}\left\{\sum_i q_i \max_{D_U}\left|\frac{\partial g_i h^{(i)}[\psi;u]}{\partial u}\right|\right\}$$

$$\delta = \frac{\pi}{2}\left\{\sum_i q_i \max_{D_U} g_i \cdot \max_{\substack{D_U \\ 0\leq\phi\leq\pi}}\left|\frac{\partial\psi(x,\Phi_i,u)}{\partial\Phi_i}\,\frac{\partial\Phi_i(u,u,n',\phi)}{\partial\phi}\right|\right\} \quad .$$

It is clear from (6.13) and (6.14) that (6.3) is satisfied provided the indicated partial derivatives remain finite.

Section 7. Stability and Convergence of Numerical Solution

Let $\psi(x,\mu,u)$ be the unique solution of (3.4), satisfying (3.10) and (3.11), in D_U. Let $W^n_{r,s}$ be the unique numerical solution of (4.14), satisfying (4.15) and (4.16), on Δ_N. The error in the numerical solution is defined, on Δ_N, as

$$(7.0) \qquad e^n_{r,s} = W^n_{r,s} - \psi(x_r,\mu_s,u_n) \cdot$$

If we define $W^n_{r+1/2,s}$ in any reasonable way (say, $= \frac{1}{2}[W^n_{r,s}+W^n_{r+1,s}]$) we have, from (3.4), (4.14), (6.0) and (6.1)

$$(7.1) \qquad \begin{aligned} \mathcal{T}[\psi(x,\mu,u)] &= 0 \quad , \quad \text{on } D_U \ ; \\ t[W^n_{r+1/2,s}] &= 0 \quad , \quad \text{on } \Delta_N \end{aligned}$$

From the linearity of these operators and the definition (7.0) we obtain, using (7.1)

$$t[e^n_{r+1/2,s}]=t[W^n_{r+1/2,s}]-t[\psi(x_r+\frac{\Delta x_r}{2},\mu_s,u_n)]$$

$$=\left\{\mathcal{T}-t\right\}[\psi(x_r+\frac{\Delta x_r}{2},\mu_s,u_n)] \quad .$$

From (6.2) the above becomes

$$(7.2) \qquad t[e^n_{r+1/2,s}] = T^n_{r,s} \quad ,$$

where the truncation is estimated in (6.13) and as outlined in the previous section may be obtained explicitly in terms of the solution, ψ, and the mesh spacing.

The errors on the boundaries, $x = 0$ and $x = a$, are easily obtained from (7.0), (4.16) and (3.10) by the methods of the previous section. We include here an inequality which results from the complete expressions:

$$(7.3) \qquad \begin{aligned} e^n_{r,s} &= 0 \qquad , \quad 0 \le s \le S_1 \ , \ n>0; \\ |e^n_{0,s}| &\le \max_{s \le S_1} |e^n_{0,s}| + (\Delta\mu)^2 \xi \ , \ S_1 < s \le S_2 \ , \ n>0; \end{aligned}$$

where $\Delta\mu$ is defined in (6.12) and $\xi \equiv \frac{1}{2} \max_{\substack{\mu<0 \\ u>0}} \left| \frac{\partial \psi(0,\mu,u)}{\partial u} \right|$.

Similarly, for the error in the highest energy solution, from (7.0), (4.15) and (3.11)

$$(7.4) \qquad \begin{aligned} e^0_{r,s} &= 0 \qquad , \quad 0 \le s \le S_1 \ , \quad 0 \le r \le R; \\ |e^0_{r,s}| &\le (\Delta x)\eta \ , \quad S_1 \le s \le S_s \ , \quad 0 \le r \le R; \end{aligned}$$

where Δx is defined in (6.12) and

$$\eta \equiv \frac{af(0)}{2\mu_* \mu_{S_1+1}} \max_{0 \le x \le a} \left| \frac{\partial \sigma^T(x,0)}{\partial x} \right| + \mathcal{O}(\Delta x)$$

To obtain bounds on the errors, $e^n_{r,s}$, we consider

(7.2) for $s \leq S_1$. In this range $\mu_s < 0$ and we obtain, using the definitions (6.1), (4.12) and (5.1),

$$(7.5) \quad e^n_{r,s} = \frac{|\mu_s| - \Delta x_r \beta(r+1,n)}{|\mu_s| + \Delta x_r \beta(r,n)} e^n_{r+1,s} + \frac{\Delta x_r/2}{|\mu_s| \Delta x_r \beta(r,n)} \left\{ \sum_i (\overline{B}^{(i)}[e^n_{r+1,s}] + \overline{B}^{(i)}[e^n_{r,s}]) + m^n_{r,s} \right\} \quad \text{for} \begin{cases} 0 \leq s \leq S_1 \\ 0 \leq n \leq N \\ 0 \leq r \leq R-1 \end{cases}$$

Let us introduce some norms of the error by

$$(7.6) \quad \begin{aligned} L_{r,n} &= \max_{0 \leq s \leq S_1} |e^n_{r,s}| , \quad R_{r,n} = \max_{S_1 \leq s \leq S_2} |e^n_{r,s}| \\ M_n &= \max_{\substack{0 \leq r \leq R \\ 0 \leq s \leq S_2}} |e^n_{r,s}| = \max_{0 \leq r \leq R} (L_{r,n}, R_{r,n}) \end{aligned}$$

Then from the definitions (4.13), (4.11) and (4.7) we have

$$(7.7) \quad \sum_i (\overline{B}^{(i)}[e^n_{r+1,s}] + \overline{B}^{(i)}[e^n_{r,s}]) \leq \Delta u G_n \sum_{n'=0}^{n-1} M_{n'} ;$$

where Δu is defined in (6.12) and we have introduced

$$(7.8) \quad G_n = 2\pi \max_{\substack{0 \leq r \leq R \\ 0 \leq n' \leq n-1}} \sum_i g_i(r,n,n') .$$

From (7.6)-(7.8) in (7.5) we obtain, taking maxima with respect to s,

$$(7.9) \quad L_{r,n} \leq \lambda_n L_{r+1,n} + \rho_n M_n ,$$

with the definitions:

$$(7.10)\quad \lambda_n = \frac{\max\limits_{r,s}\left|\,|\mu_s| - \Delta x_r \beta(r+1,n)\right|}{\min\limits_{r,s}\left|\,|\mu_s| + \Delta x_r \beta(r,n)\right|},$$

$$\rho_n \equiv \frac{\Delta x/2}{\min\limits_{r,s}\left|\,|\mu_s| + \Delta x_r \beta(r,n)\right|},$$

$$T_n \equiv \max_{r,s}|T^n_{r,s}|E_n \equiv \Delta u G_n \sum_{n'=0}^{n-1} M_{n'} + T_n .$$

Applying (7.9) recursively yields

$$(7.11)\qquad L_{r,n} \le (\lambda_n)^{R-r} L_{R,n} + \frac{1-(\lambda_n)^{R-r}}{1-\lambda_n}\rho_n E_n .$$

In an exactly analogous manner we obtain, by considering (7.2) for $s > S_1$,

$$(7.12)\qquad R_{r,n} \le (\Lambda_n)^r R_{0,n} + \frac{1-(\Lambda_n)^r}{1-\Lambda_n} P_n E_n ,$$

where

$$(7.13)\quad \Lambda_n = \frac{\max\limits_{r,s}\left|\,|\mu_s| - \Delta x_r \beta(r,n)\right|}{\min\limits_{r,s}\left|\,|\mu_s| + \Delta x_r \beta(r+1,n)\right|},\quad P_n = \frac{\Delta x/2}{\min\limits_{r,s}\left|\,|\mu_s| + \Delta x_r \beta(r+1,n)\right|} .$$

The first term on the right in (7.12) indicates the propagation of errors introduced at the boundary $x = 0$. A similar remark applies, in (7.11), to the errors introduced at the boundary $x = a$. These errors would actually be damped if $|\lambda_n| < 1$ and $|\Lambda_n| < 1$. The errors due to truncation

and those introduced at the mamimum energy are propagated in the terms containing E_n.

From (7.3) we deduce, using (7.6),

$$L_{R,n} = 0$$

(7.14)

$$R_{0,n} \leq L_{0,n} + (\Delta\mu)^2\xi \ .$$

Now (7.11) and (7.12) become

$$L_{r,n} \leq [\frac{1-(\lambda_n)^{R-r}}{1-\lambda_n}\rho_n]E_n$$

(7.15)

$$R_{r,n} \leq [(\Lambda_n)^r\frac{1-(\lambda_n)^R}{1-\lambda_n}\rho_n + \frac{1-(\Lambda_n)^r}{1-\Lambda_n}P_n]E_n + (\Lambda_n)^r(\Delta\mu)^2\xi$$

From (7.10) and (7.13) we see that in a shield of piecewise-constant composition: $\lambda_n \equiv \Lambda_n \equiv \bar{\lambda}_n$ and $\rho_n \equiv P_n = \bar{\rho}_n$, say, and (7.15) becomes

$$L_{r,n} \leq [\frac{1-(\bar{\lambda}_n)^{R-r}}{1-\lambda_n}\bar{\rho}_n]E_n$$

(7.16)

$$R_{r,n} \leq [\frac{1-(\bar{\lambda}_n)^{R+r}}{1-\lambda_n}\bar{\rho}_n]E_n + (\bar{\lambda}_n)^r(\Delta\mu)^2\xi \ .$$

In general it is easy to show that the above equations are valid if $\bar{\lambda}_n$ and $\bar{\rho}_n$ are defined as

$$\bar{\lambda}_n = \frac{\max\limits_{r,s}\left\{\left||\mu_s|-\Delta x_r\beta(r+1,n)\right|, \left||\mu_s|-\Delta x_r\beta(r,n)\right|\right\}}{\min\limits_{r,s}\left\{\left||\mu_s|+\Delta x_r\beta(r,n)\right|, \left||\mu_s|+\Delta x_r\beta(r+1,n)\right|\right\}} \geq \max(\lambda_n, \Lambda_n)$$

(7.17)

$$\bar{\rho}_n = \frac{\Delta x/2}{\min\limits_{r,s}\left\{\left||\mu_s|+\Delta x_r\beta(r,n)\right|, \left||\mu_s|+\Delta x_r\beta(r+1,n)\right|\right\}} = \max(\rho_n, P_n) \ .$$

Taking the maximum in (7.16) with respect to r and recalling definitions (7.6) yields an inequality of the form

$$M_n \leq \Theta_n E_n + (\Delta\mu)^2\xi \times \max[1, (\bar{\lambda}_n)^R],$$

where

$$\Theta_n \equiv \max_{0\leq r\leq R} \frac{\bar{\rho}_n}{1-\bar{\lambda}_n}[1-(\bar{\lambda}_n)^{R-r}, 1-(\bar{\lambda}_n)^{R+r}] .$$

Without loss of generality we may assume $\bar{\lambda}_n \leq 1$ in which case these relations become

(7.18)

a) $M_n \leq \Theta_n E_n + (\Delta\mu)^2\xi$,

b) $\Theta_n = \dfrac{1-(\bar{\lambda}_n)^{2R}}{1-\bar{\lambda}_n}\bar{\rho}_n$.

From (7.10) in the above inequality we have

$$M_n \leq \Delta\mu\Theta_n G_n \sum_{n'=0}^{n-1} M_{n'} + \Theta_n T_n + \Delta\mu^2\xi ,$$

or

$$M_n \leq \Delta\mu K_n \sum_{n'=0}^{n-1} M_{n'} + F_n , \tag{7.19}$$

where we have introduced:

(7.20)

a) $K_n \equiv \max_{n'\leq n} \Theta_{n'} G_{n'}$

b) $F_n \equiv \max_{n'\leq n} \Theta_{n'} T_{n'} + \Delta\mu^2\xi$.

With these definitions we easily obtain from a recursive

application of (7.19)

$$(7.21) \qquad M_n \leq (1+\Delta\mu K_n)^{n-1}[\Delta\mu K_n M_0 + F_n] \ .$$

A well known inequality states that

$$(7.22) \qquad (1+\frac{k}{n})^n < e^k$$

for $k \geq 0$ and all positive integers, n . Thus if the lethargy spacing were equal, say $n\Delta u = u_n$, we would have by the above inequality

$$(1+\Delta u K_n)^{n-1} < e^{K_n u_{n-1}} \qquad .$$

For arbitrary spacing, as used in the present scheme, there exists for each value of $n \leq N$ a bounded number, $t_{n,N}$, such that

$$(7.23) \qquad \Delta u = \frac{u_n}{n} t_{n,N} \ , \ 1 \leq t_{n,N} < \infty \ ;$$

where we recall $\Delta u \equiv \max_{0 \leq n < N} \Delta u_n$. Thus in general

$$(7.24) \qquad (1+\Delta u K_n)^{n-1} < e^{K_n u_{n-1} t_{n-1,N}} \qquad ;$$

and (7.21) implies

$$(7.25) \qquad M_n < e^{K_n u_{n-1} t_{n-1,N}}[\Delta u K_n M_0 + F_n]$$

From (7.4) and (7.6) we have

$$(7.26) \qquad M_0 \leq (\Delta x)\,\eta \qquad .$$

From (7.20)b), (7.10) and the estimate (6.13) we have

$$(7.27)\quad F_n \leq \theta\left\{(\Delta x)^2\alpha+(\Delta\mu)^2\beta+(\Delta u)\gamma+(\Delta\phi)\delta+\sigma((\Delta u)^2+(\Delta\phi)^2)\right\} + (\Delta\mu)^2\xi ,$$

where

$$(7.28)\qquad \theta \equiv \max_{n\leq N} \theta_n \quad .$$

Thus the final form of (7.25) may be written as

$$(7.29)\quad M_n < e^{K_n u_{n-1} t_{n-1,N}}[(\Delta u)(\Delta x)K_n\eta+\theta\left\{(\Delta x)^2\alpha+(\Delta\mu)^2\beta+ +(\Delta u)\gamma+(\Delta\phi)\delta+\sigma((\Delta u)^2+(\Delta\phi)^2)\right\}+(\Delta\mu)^2\xi] \ .$$

We now assume that the mesh, Δ_N, satisfies conditions (5.7) and (5.8). Then the inequalities (5.3) hold and the absolute value signs may be dropped in the definitions (7.17). Since the denominators in $\bar{\lambda}_n$ and $\bar{\rho}_n$ are evaluated for the same values of r and s, say r', s', we have

$$(7.30)\quad \frac{\bar{\rho}_n}{1-\bar{\lambda}_n} = \frac{\Delta x}{2\left\{\mu_{s'}+\Delta x_{r'}\beta(r',n)-\mu_{s''}+\Delta x_{r''}\beta(r'',n)\right.} ,$$

$$= \frac{1}{2\left\{\frac{\mu'_s}{\Delta x} - \frac{\mu_{s''}}{\Delta x} + \frac{\Delta x_{r'}}{\Delta x}\beta(r',n) + \frac{\Delta x_{r''}}{\Delta x}\beta(r'',n)\right.})$$

where r'', s'' are the integers for which the numerator in $\bar{\lambda}_n$ is a maximum. For simplicity we have written the $\beta(r,n)$ at $r = r'$ and r''. These could be replaced by the values at $r = r' + 1$ or $r = r'' + 1$, as the case may be,

with no change in the following. The conditions imposed on the mesh insure that $\bar{\lambda}_n<1$ and hence for such mesh spacing the denominator in (7.30) never vanishes.

The methods used to derive (7.24) yield, when applied to the definition (7.17)

$$(7.31)\quad 1-(\bar{\lambda}_n)^{2R}<1-\exp\left\{-\left[\frac{\Delta x_{r'}}{|\mu_{s'}|}\tilde{\zeta}_{r',R}\beta(r',n)+\frac{\Delta x_{r''}}{|\mu_{s''}|}\tilde{\zeta}_{r'',R}\beta(r'',n)\right][2a]\right\}$$

Here r', r'', s' and s'' are defined in the previous paragraph and as in (7.23) we have introduced the bounded positive constants $\tilde{\zeta}_{r',R}$ such that:

$$(7.32)\qquad \Delta x_{r'} = \frac{a}{R}\tilde{\zeta}_{r',R} \quad ,$$

Condition (5.7) insures that the $\beta(r',n)$ are ≥ 0 and thus the exponential in (7.31) is bounded for all possible $\mu_{s'}$. From (7.28), (7.18)b), (7.30) and (7.31) we have

$$(7.33)\quad \theta<\left(1-\exp\left\{-\left[\frac{\Delta x_{r'}}{|\mu_{s'}|}\tilde{\zeta}_{r',R}\beta(r',n)+\frac{\Delta x_{r''}}{|\mu_{s''}|}\tilde{\zeta}_{r'',R}\beta(r'',n)\right][2a]\right\}\right)\cdot\frac{1}{2}\left\{\frac{\mu_{s'}}{\Delta x}-\frac{\mu_{s''}}{\Delta x}+\frac{\Delta x_{r'}}{\Delta x}\beta(r',n)+\frac{\Delta x_{r''}}{\Delta x}\beta(r'',n)\right\}^{-1}$$

for some $n\leq N$. However, by (7.20a) and (7.8)

(7.34) $\qquad K_n < \Theta 2\pi \sum g_1(r'', n', n'')$

for some r'' and $n'' < n' \leq n$. Thus K_n and Θ are bounded for all meshes Δ_N satisfying (5.7) and (5.8). The constants α, β, γ, δ defined in (6.14), η defined after (7.4) and ξ defined after (7.3) are bounded independent of the mesh spacing. Thus the errors $|e^n_{r,s}|$, which are bounded by $\max_n M_n$ of (7.29), tend to zero with the mesh spacing, $\Delta x \longrightarrow 0$, $\Delta u \longrightarrow 0$, $\Delta \mu \longrightarrow 0$ and $\Delta \phi \longrightarrow 0$; provided conditions (5.7) and (5.8) are satisfied. Hence the numerical solutions $W^n_{r,s}$ converge uniformly to the solution $\psi(r, \mu, u)$ in D_U on an appropriate sequence of meshes Δ_N. The stability and convergence of the proposed difference scheme are thus demonstrated.

References

[1] R. E. Marshak; Theory of the Slowing Down of Neutrons by Elastic Collision with Atomic Nuclei, Rev. Mod. Phys., 19 (3), 1947 (185-238).

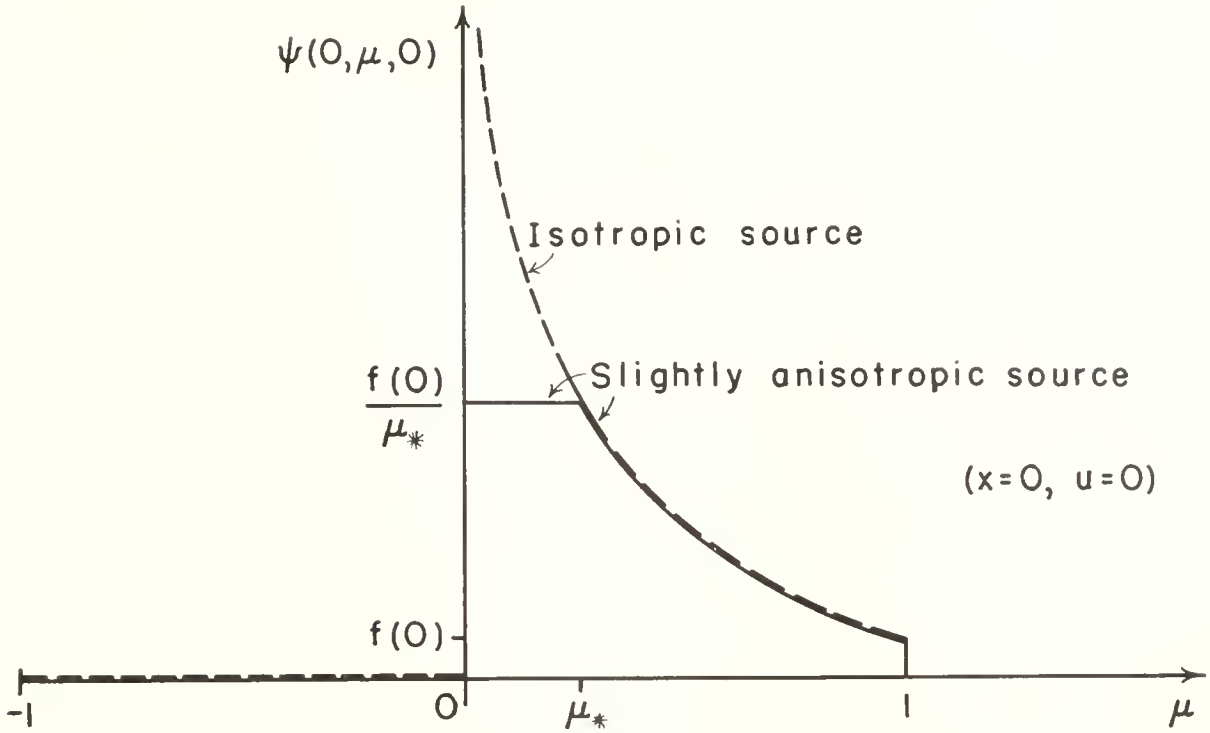

Figure I

Maximum Energy Solutions in the Source Plane

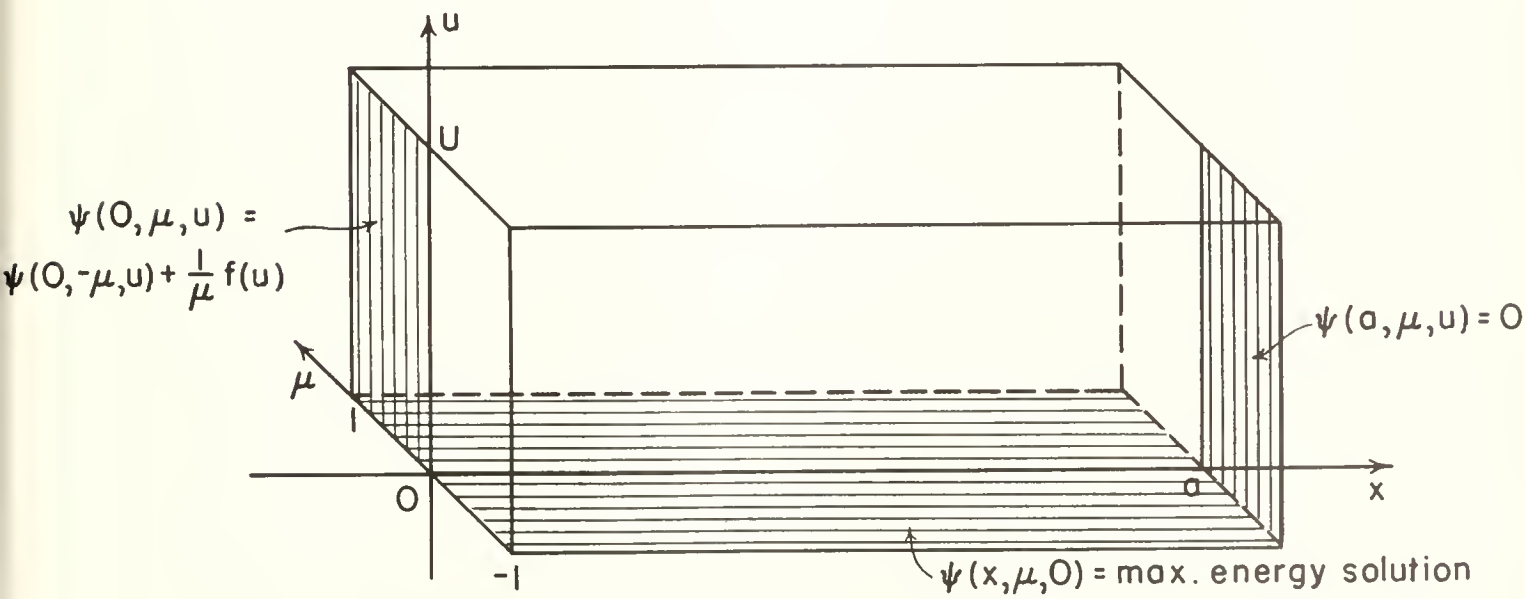

Figure II

The Domain D with Indicated Boundary and Initial Conditions

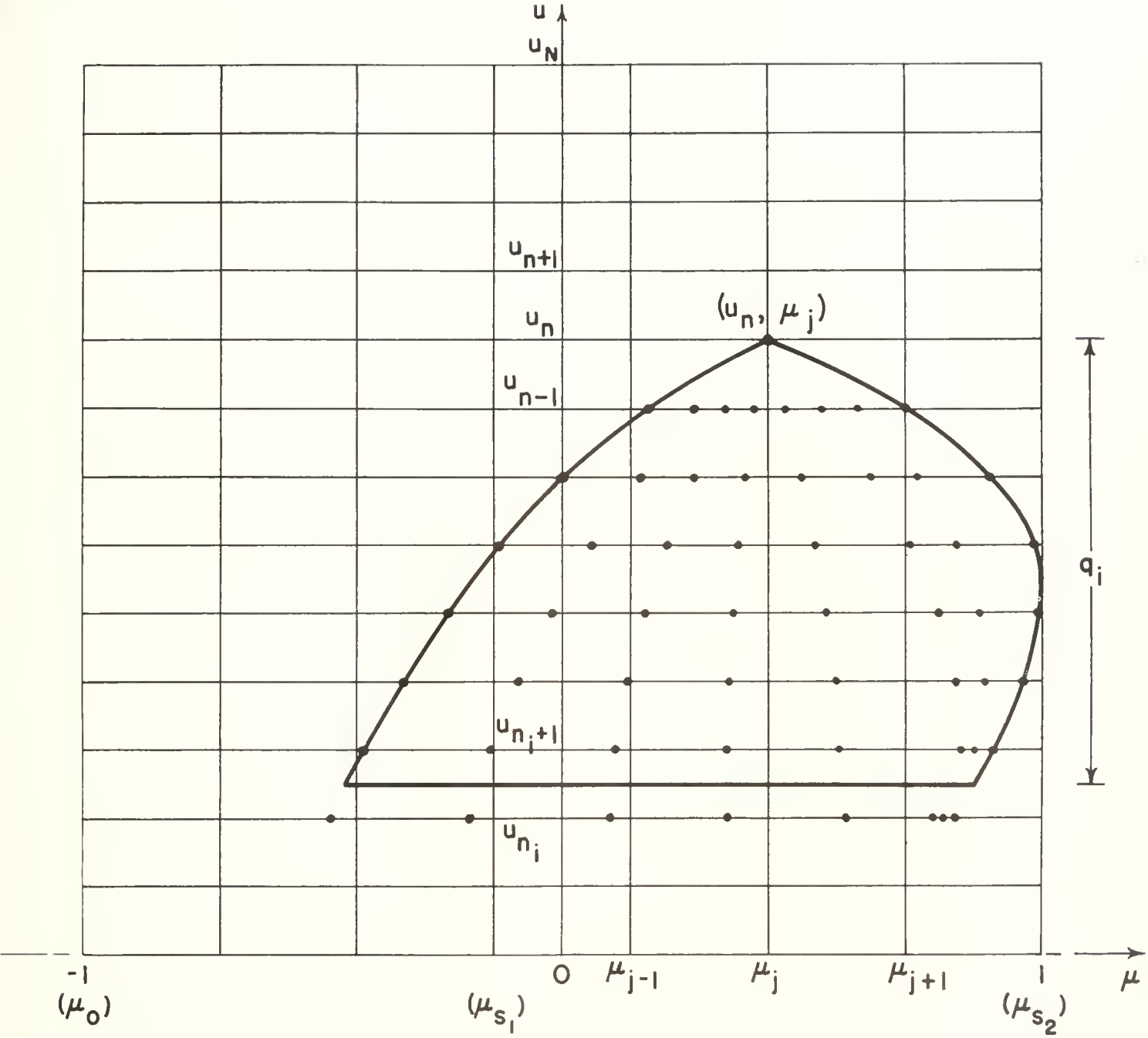

Figure III

Domain of Integration for i-th Birth Integral $b^i[\psi]$ at $u = u_n$, $\mu = \mu_j$ in Some Plane $x = x_r$.

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On the numerical integration of the neutron transport equation.